Multiscale Modeling of Electronic Materials CRA

Dr. Martin Berzins
Program Manager

Dr. Meredith Reed
Collaborative Alliance Manager

MSME/MEDE kick-off meeting 31 July, 2012

Current Electronic Devices for Army Battlefield Superiority

Future Capabilities

will rely on the ability to specifically design materials for continued

Army Soldier superiority on the battlefield

Why Multiscale Modeling of Electronic Materials?

Materials by Design

Validated multiscale & multidisciplinary modeling capability to apriori predict material structure, properties, and performance.

Three Electronic Materials Research Areas:

- Electrochemical Energy Materials
- Hybrid Photonics Materials
- Heterogeneous Metamorphic Electronic Materials

Provide the US Army with:

- New materials and devices with unprecedented properties and capabilities
- Strategic advantage for investing and developing materials for current/future war fighter
- Reduce development time and cost
- Improved and enabling materials/systems that are in line with TeCD goals (e.g., Force Protection, Overburden, Tactical Intelligence, Sustainability/Logistics, etc.)

FUTURE PAYOFFS

Materials by Design

Provide an Enterprise for Innovation

Empower Unburden and Protect

Sensors, Devices, Power and Energy

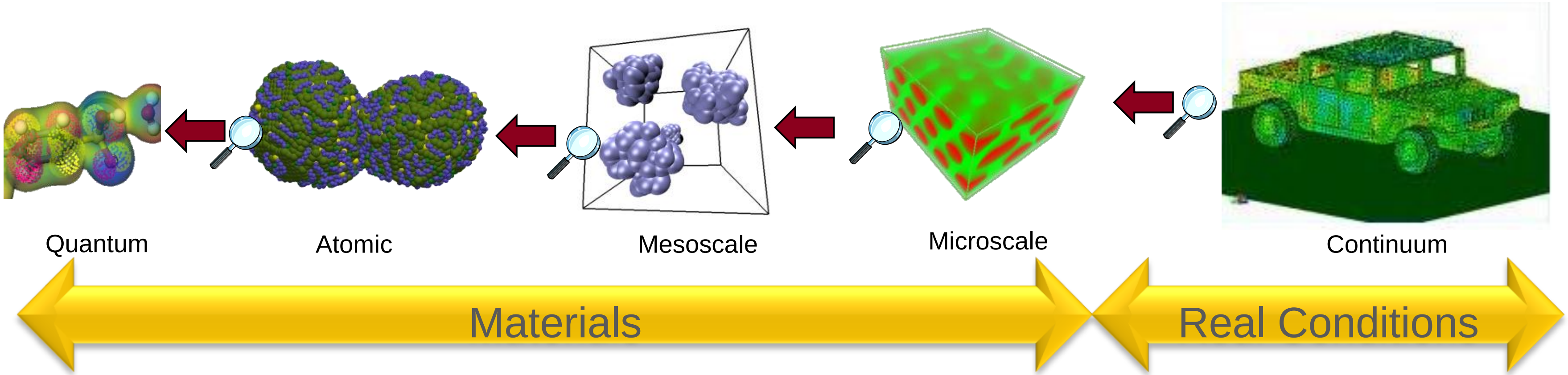
3X in energy density
30% more efficient
30% longer lifetimes

Vehicle and Soldier Protection

1/3 savings in weight

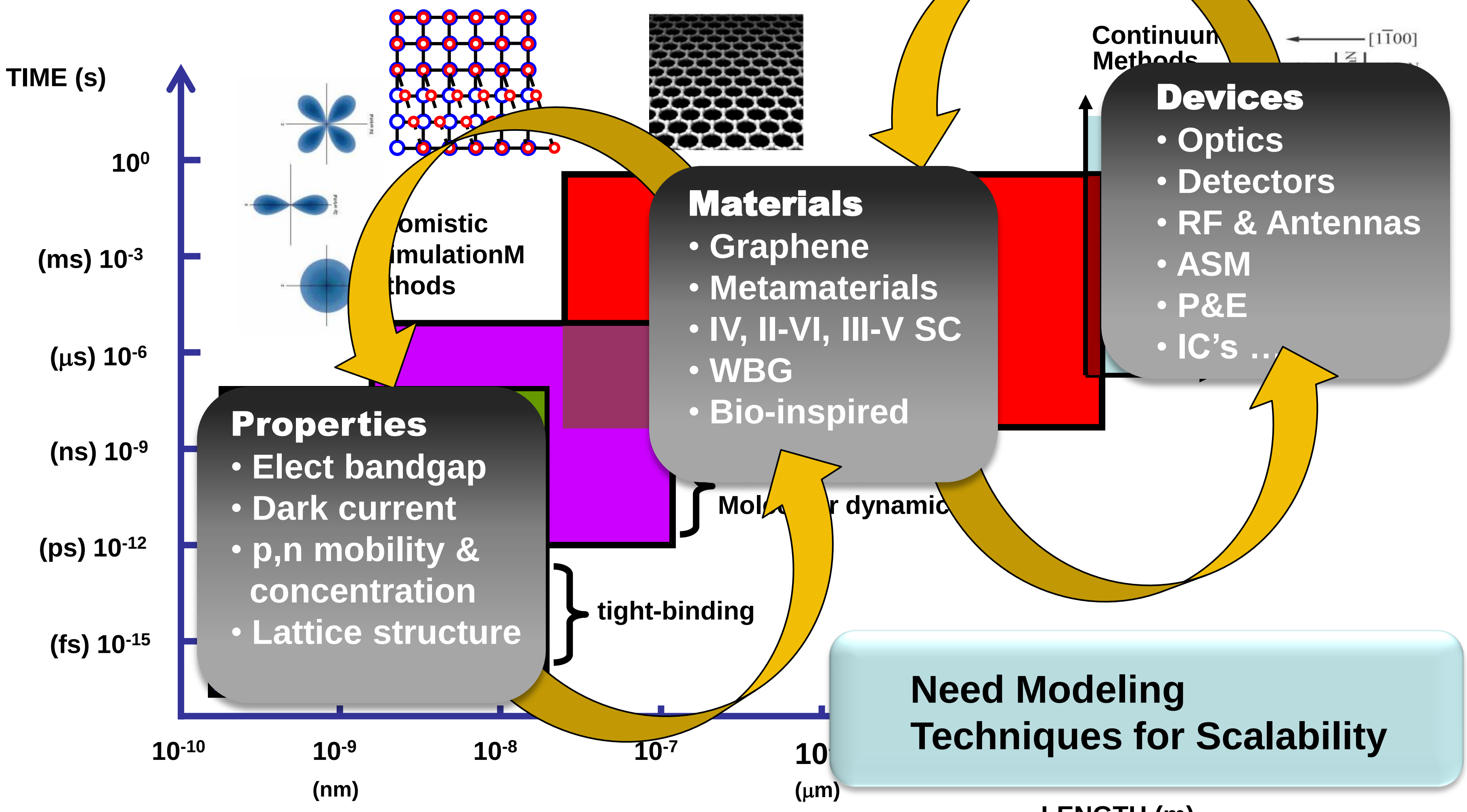
Why Now?

- Discovery of new materials (e.g. graphene, metamaterials, plasmonics, high voltage cathodes …)
- Need understanding and guidance for new or improved material development
- Multi-core processors → Petascale, Exascale, Graphical Processing Units (GPUs)
- Support maturation of electronic materials (IR, nano, e.g. CNT, WBG)
- Advancements in UQ and V&V



Multiscale Modeling of Electronic Materials

Challenge: Modeling a physical phenomenon from a broad range of perspectives, from the atomistic to the macroscopic end



Multiscale Modeling of Electronic Materials

Strategic Directions
- Devices for Networks
- Persistent Surveillance
- Unique electronics for BS effects, sensing & processing
- Ubiquitous Efficient Energy

Sensors
- IRSTA
- Nav
- PS/SA
- FC

Devices
- Optics
- Detectors
- RF & Antennas
- ASM
- P&E
- IC's …

Materials
- Graphene
- Metamaterials
- IV, II-VI, III-V SC
- WBG
- Bio-inspired

Properties
- Elect bandgap
- Dark current
- p,n mobility & concentration
- Lattice structure

Atomic Structure

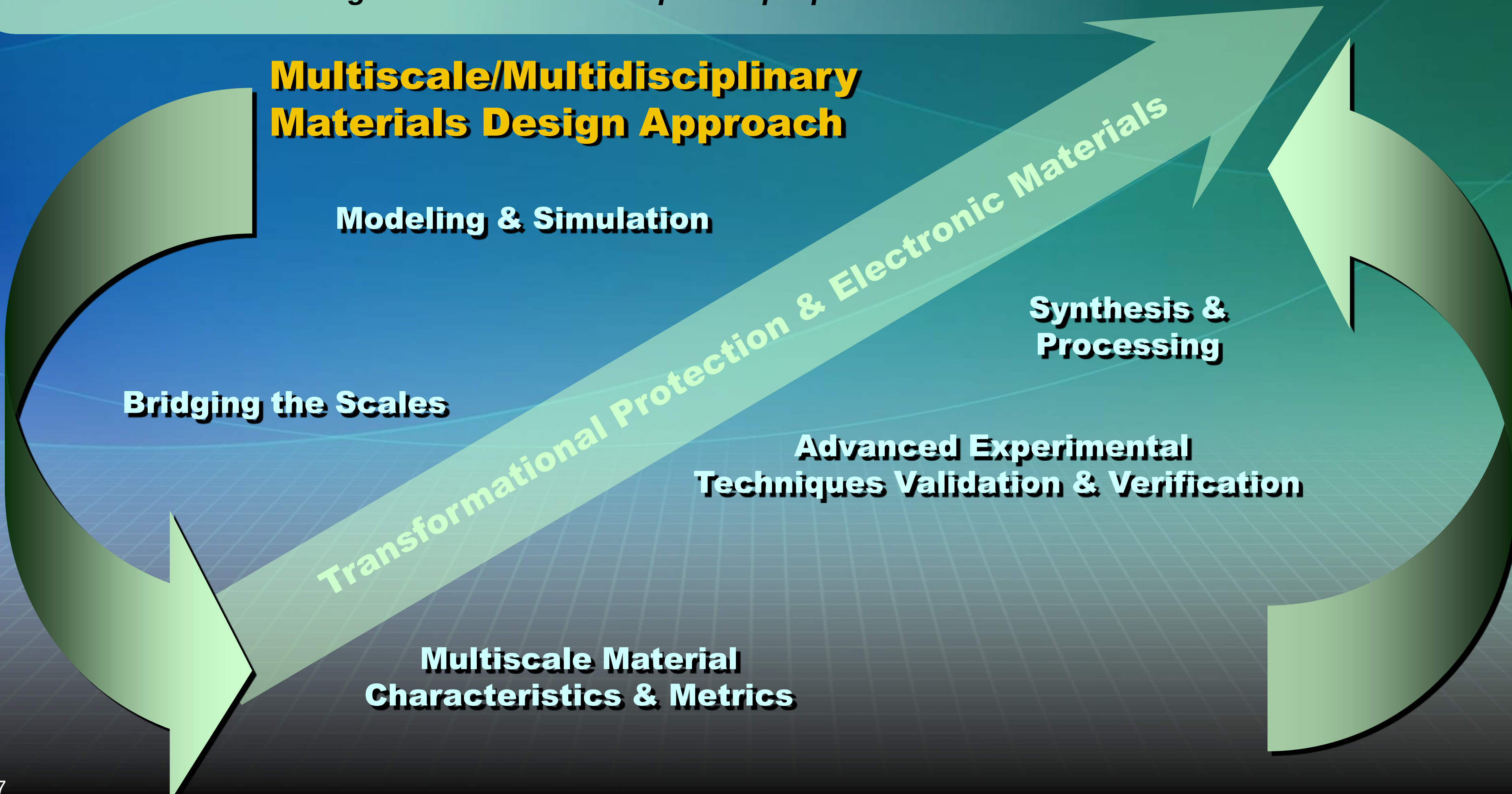
Multi-Scale Effects from Surfaces, Interfaces & Defects

Materials Models Must Be Multi-Scale

APPROACH

Fundamental research with a "materials by design" approach to relate the response of structural and electronic materials across critical length & time scales to specific properties

Electronic and Protection Materials for U.S. Army Systems



Performed for each of the Electronic Materials Research Areas

Experimental Analysis Characterization

External CRA Effort

Computational Techniques

Computational Techniques

- **Modeling and Simulation:** Validated multiscale modeling of electronic materials design materials and predict performance by exploiting the hierarchy of scales in a multidisciplinary environment
- **Bridging the Scales: Analysis, Theory and Algorithms:** Validated theoretical and analytical analyses to effectively define the interface physics across length scales and disciplines
- **Multiscale Modeling Material Metrics:** A comprehensive set of metrics that electronic material for each of the three Electronic Materials Research Areas defined above to enable the enhancement or creation of new electronic devices
- **Validation and Verification:** Comprehensive validated experimental capabilities bridging time and space for probing the physics and mechanisms of electronic materials and for verification and validation of multiscale/multidisciplinary physics modeling.
- **Synthesis and Processing:** Validated modeling and techniques for the synthesis and processing of Electronic Materials.

US ARMY RDECOM

MSME Crosscutting Themes

ARL

Electrochemistry

Focus on interfacial physics and chemistry; nano structures, solid-liquid interface–clear opportunities for batteries, fuel cells, etc.

Hybrid Photonics

Interaction of photons, electrons, phonons–photonics, spintronics, plasmonics, and phonons

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Heterogeneous Metamorphic Electronics

Mixed materials, with partial ordering–includes graphene, metamaterials, nanoelectronic structures, etc.

Develop fundamental understanding and computational techniques for a broad base of materials

Cross-cutting Materials and Modeling Challenges

- **Verification and Validation/Uncertainty Quantification**
- **Bridging scales:**
  - Coarse graining
  - Adaptive mesh refinement
- **Transport:**
  - At/across interfaces
  - Electron or photon transport
  - Energy transport
  - Mass/ion transport
- **Defects:**
  - Defects, surfaces or interfaces
  - Strain
  - Impurities, Vacancies, Interstitials
  - Point Defects
  - Compositional inhomogeneities

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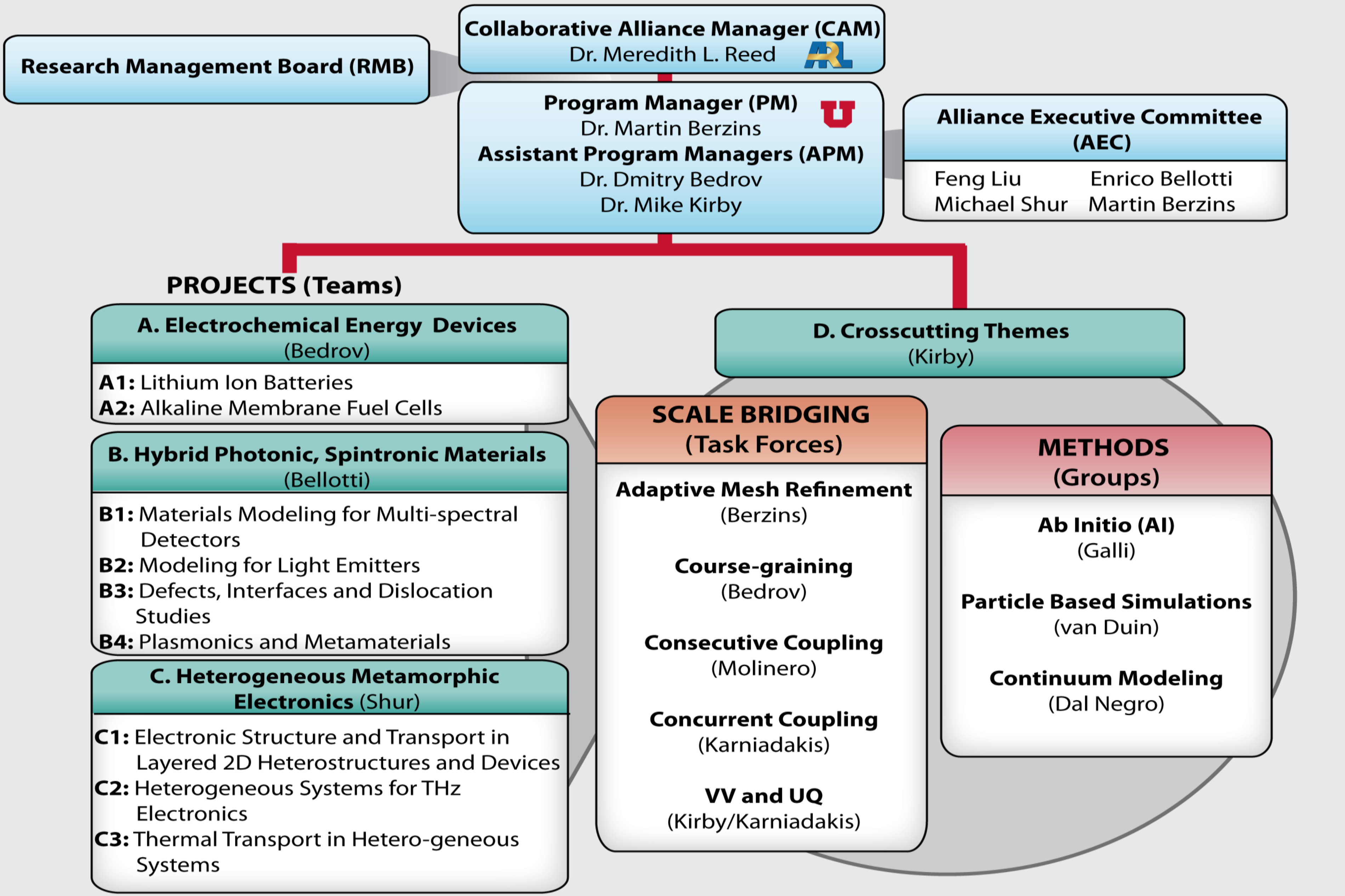
Computationally-guided Design of Energy Efficient Electronic Materials (CDE_3M) Organizational Chart



ARL Team/Collaboration with MSME CRA

CAM: Meredith Reed

TECHNICAL LEADS

ARL Scientists/Collaborators
(both modelers and experimentalists)

Cross-cutting Collaboration

Electrochemistry
- Oleg Borodin (Batteries)
- Kyle Grew (Fuel Cells)

Richard Jow
Cindy Lundgren
Deryn Chu
Jan Allen

Heterogeneous Metamorphic
- Terrance O'Regan

Frank Crowne
Pankaj Shah
Madan Dubey
Glen Birdwell
Amir Zaghloul
Steve Weiss

Hybrid Photonics
- Sergey Rudin

Greg Rupper
Priyalal Wijewarnasuriya
Michael Wraback
Greg Garrett
Anand Sampath
Ken Jones
Randy Tomkins
Greg Brill
Grace Metcalfe

Cross-cutting Materials and Computational Themes for Materials by Design

Transport | Defects | Bridging Scales

Team Members ARL/University of Utah Collaborative Research Alliance

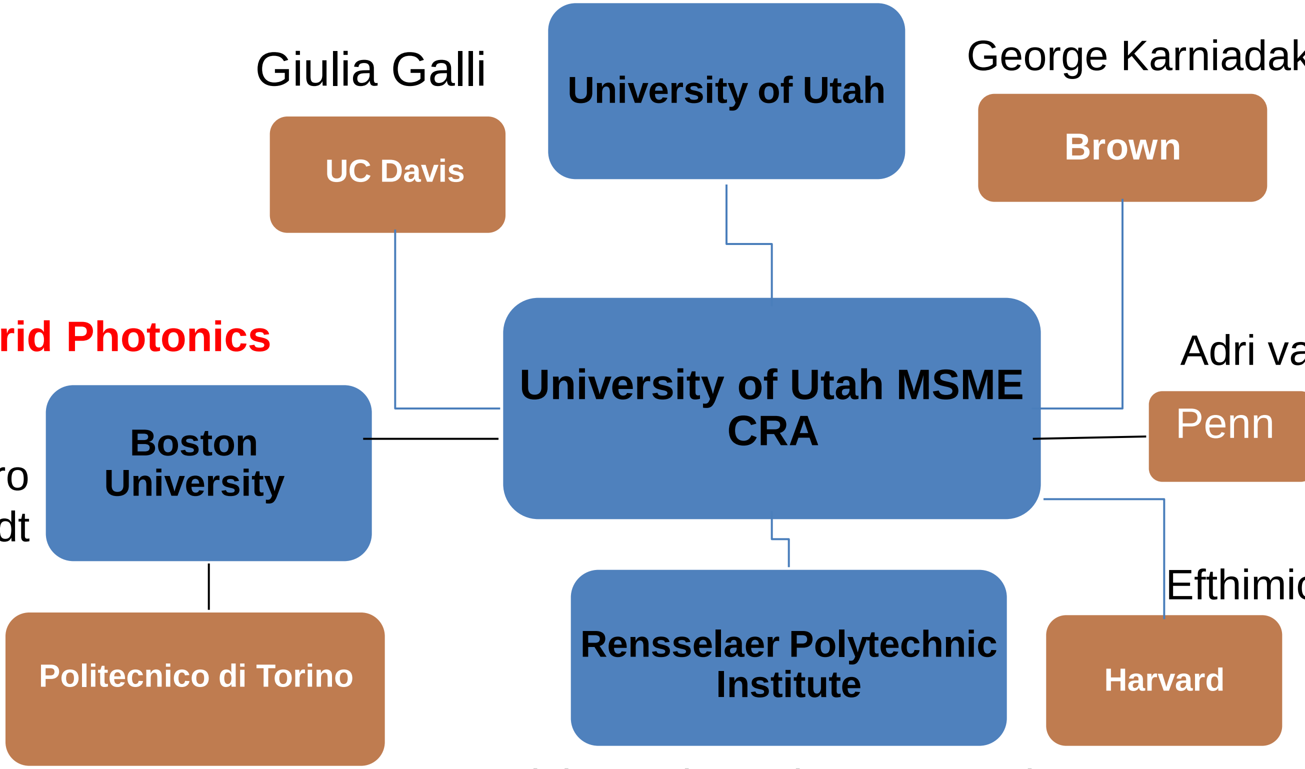
Spend About $3M per year including cost share

Dmitry Bedrov
Martin Berzins
Feng Liu
Mike Kirby
Valeria Molinaro

Area A: Electrochemical Energy

Giulia Galli

George Karniadakis



Adri van Duin

Area B :Hybrid Photonics

Enrico Bellotti
Luca Del Negro
Martin Herbordt

Efthimios (Tim) Kaxiras

Giuseppi Vecchi
Francesco Bertazzi

Michael Shur, Vincent Meunier ,
Saroj Nayak, Pawel Koblinsky,

Area C: Heterogeneous Metamorphic Electronics

Multiscale Modeling of Electronic Materials (MSME) Collaborative Alliance Members

LRO: University of Utah

Program Manager: Martin Berzins
Professor School of Computing and SCI Institute Scale Bridging, Adaptive Mesh Refinement

Assistant Program Managers :
Dmitry Bedrov Research Associate Professor Materials
Mike Kirby Associate Professor School of Computing and SCI Institute

Rensselaer Polytechnic Institute (RPI)

Principal: Michael S. Shur
Professor of Electrical, Computer and Systems Engineering, and Professor of Physics , Applied Physics and Astronomy
Director, NSF RPI Connection One I/UCRC Center
Heterogeneous Metamorphic Electronics

Boston University

Principal: Enrico Bellotti
Associate Professor of Electrical and Computer Engineering Department
Director, Computational Electronics Laboratory (CEL)
Hybrid Photonics Materials

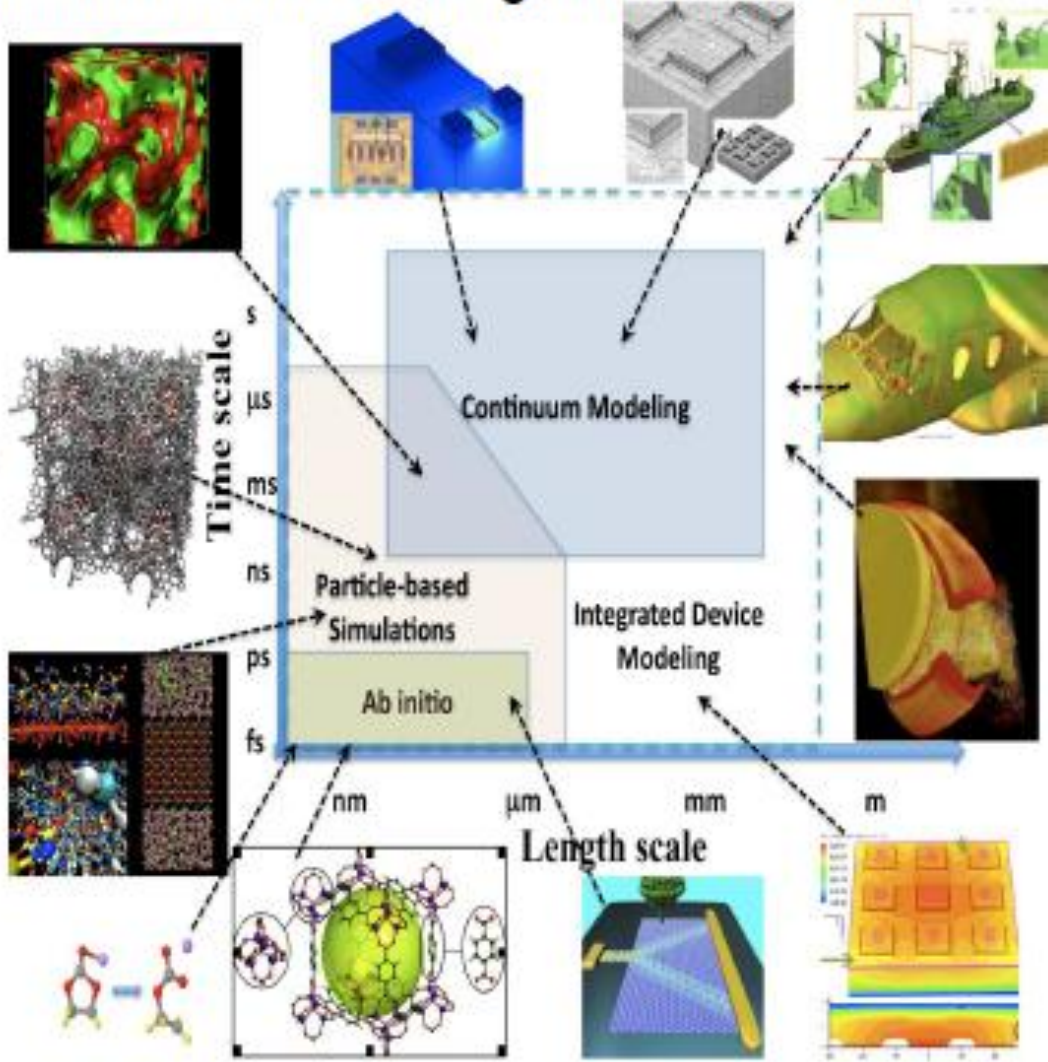
US Army Research Laboratory

Collaborative Alliance Manager: Meredith L. Reed

ARL brings expertise in electronic, electro-optical and electrochemical materials and devices design, modeling, synthesis and processing, characterization, multiscale modeling and computational tool development.

State of the Art in Simulation and MSME

Advances in MSME application areas require not only **fundamental materials research** but application of cross-cutting **multiscale and multidisciplinary** methods.



Outline:

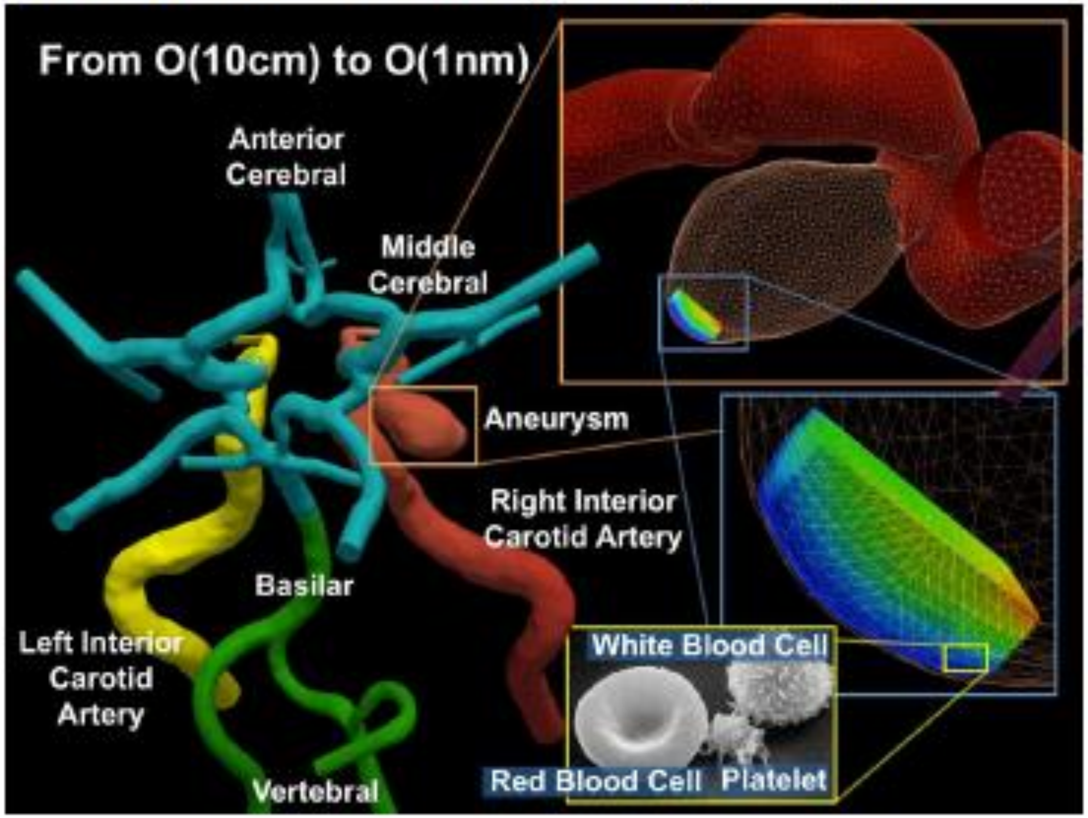
The state of the art in multi-scale modeling and VVUQ

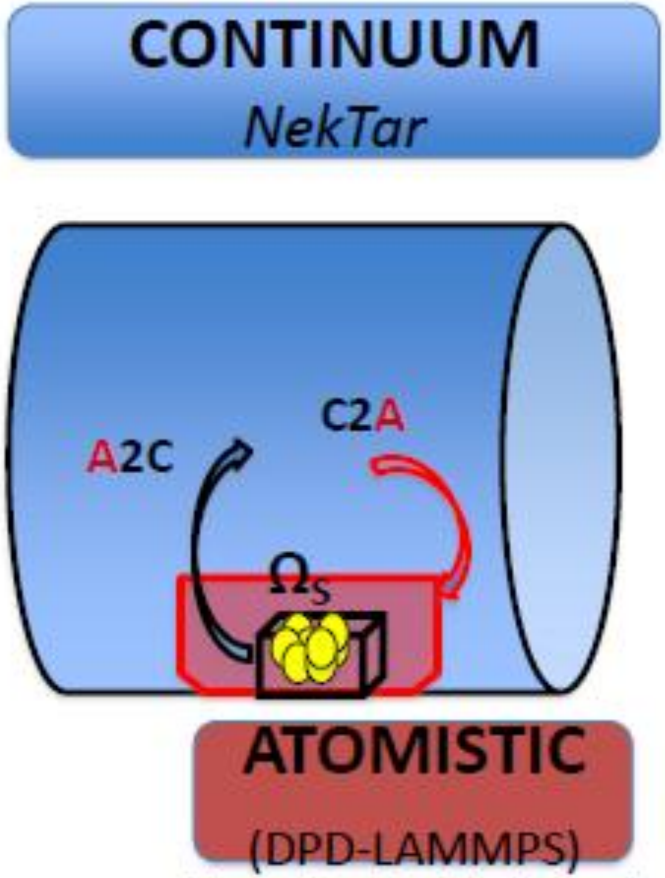
Overview of three materials areas (Bedrov, Bellottii and Shur) and cross-cutting methods (Kirby Galli).

Detailed material applications Wednesday AM

State of the Art in Multiscale Modeling

Interfacing MD models of platelets with continuum models of blood flow in modeling aneurysm rupture - Grinberg and Karniadakis



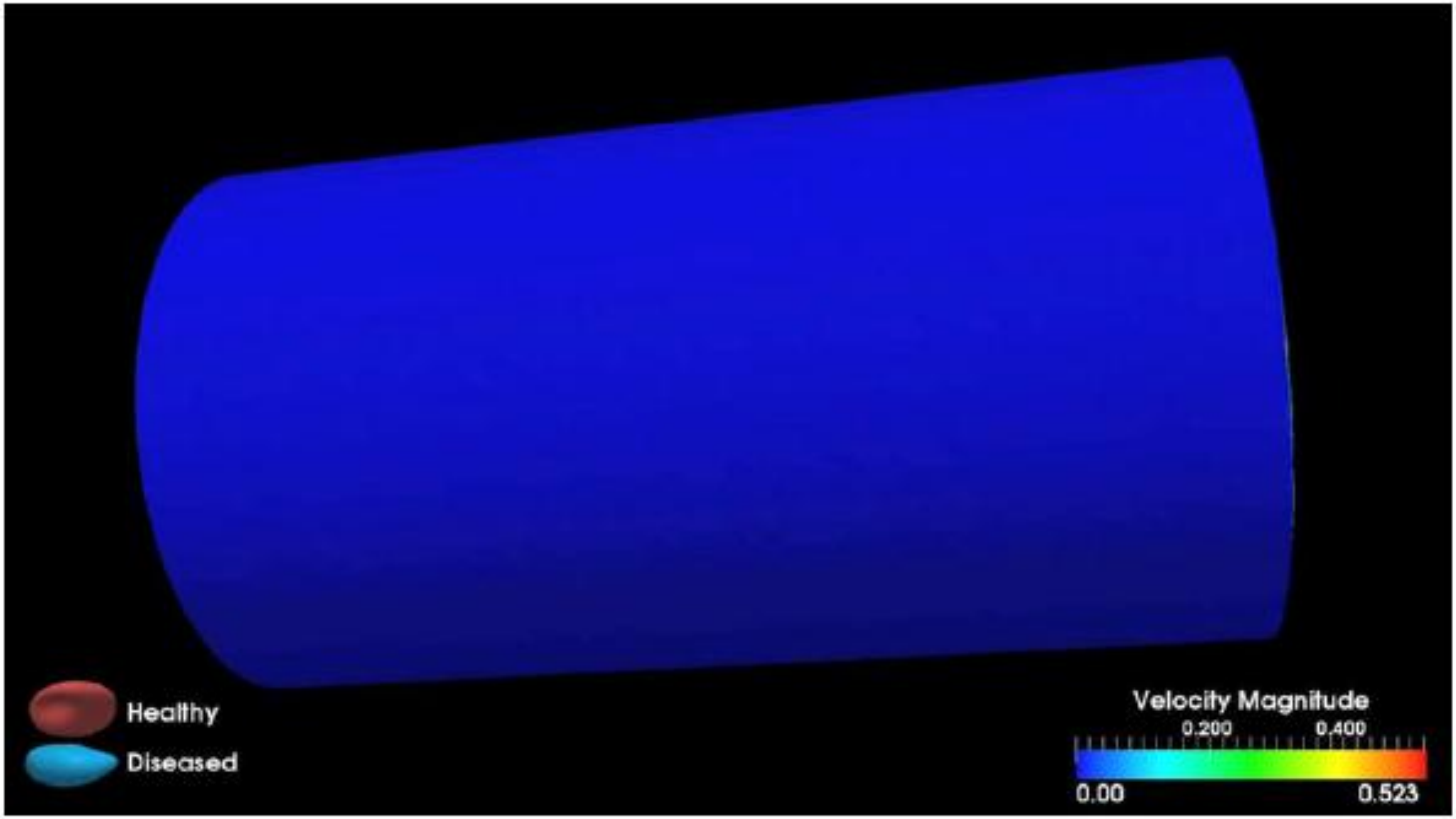


Platelet model in atomistic domain Ω_S

A2C are atomistic to continuum boundary conditions

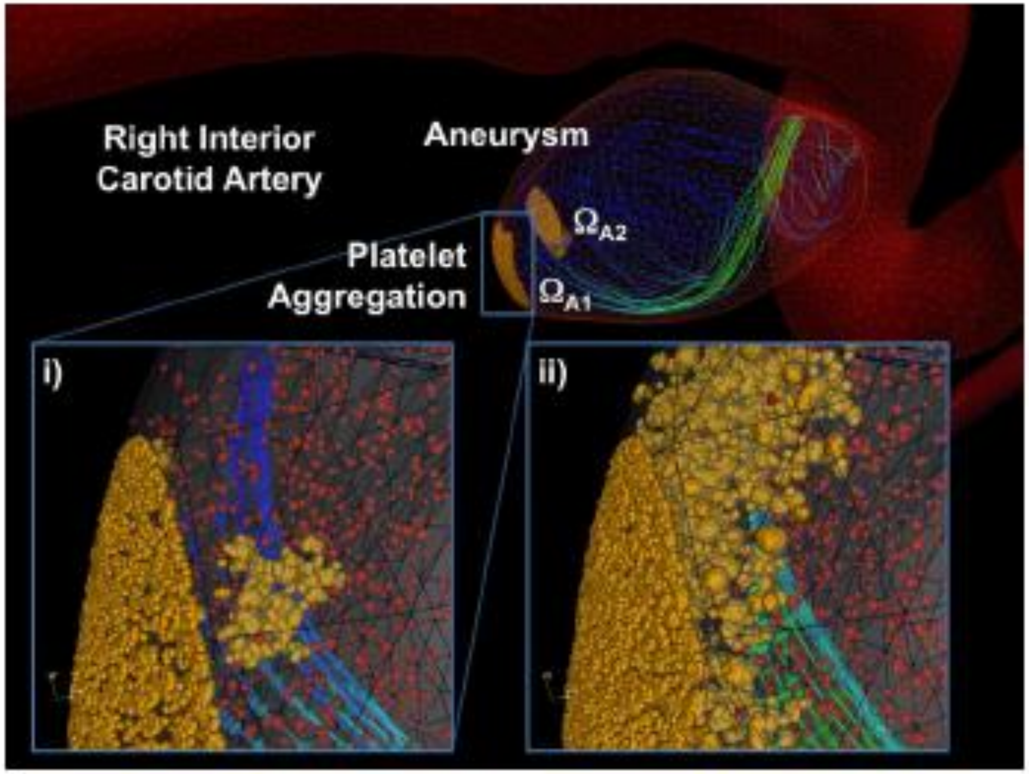
Dissipative Particle Dynamics particles are agglomerations of MD particles

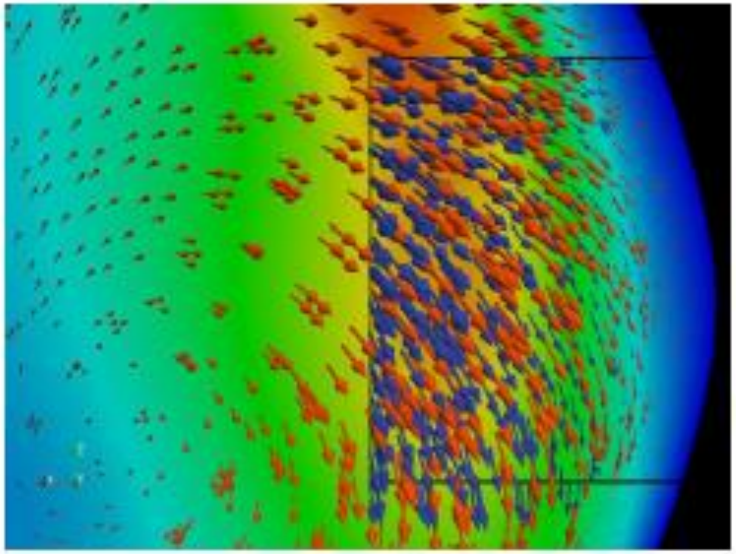
Multiscale Model including Continuum Atomistic DPD interactions



Source Leo Grinberg

Results Velocities Scaling





Continuum velocities

Particle Velocities

Clot Formation

Progression of clot

Yellow dots are active platelets, red dots are inactive platelets

Ncore (DPD-LAMMPS+Nektar)	CPU-time for 4000 steps	Speedup
8 Racks (32,768 cores)	7952 s	1.0
72 Racks (294,912 cores)	733 s	10.85

JÜLICH FORSCHUNGSZENTRUM Parallel Computing

Grinberg and Karniadakis

In Modeling and Simulation you don't know how good (or bad) you are if you don't ask.

We now compute very complex solutions to ever more challenging computational modeling problems. **Due diligence requires that we ask**:

How accurate is the model that we use?

How accurate is the solution to that model?

How does the solution vary if the model does?

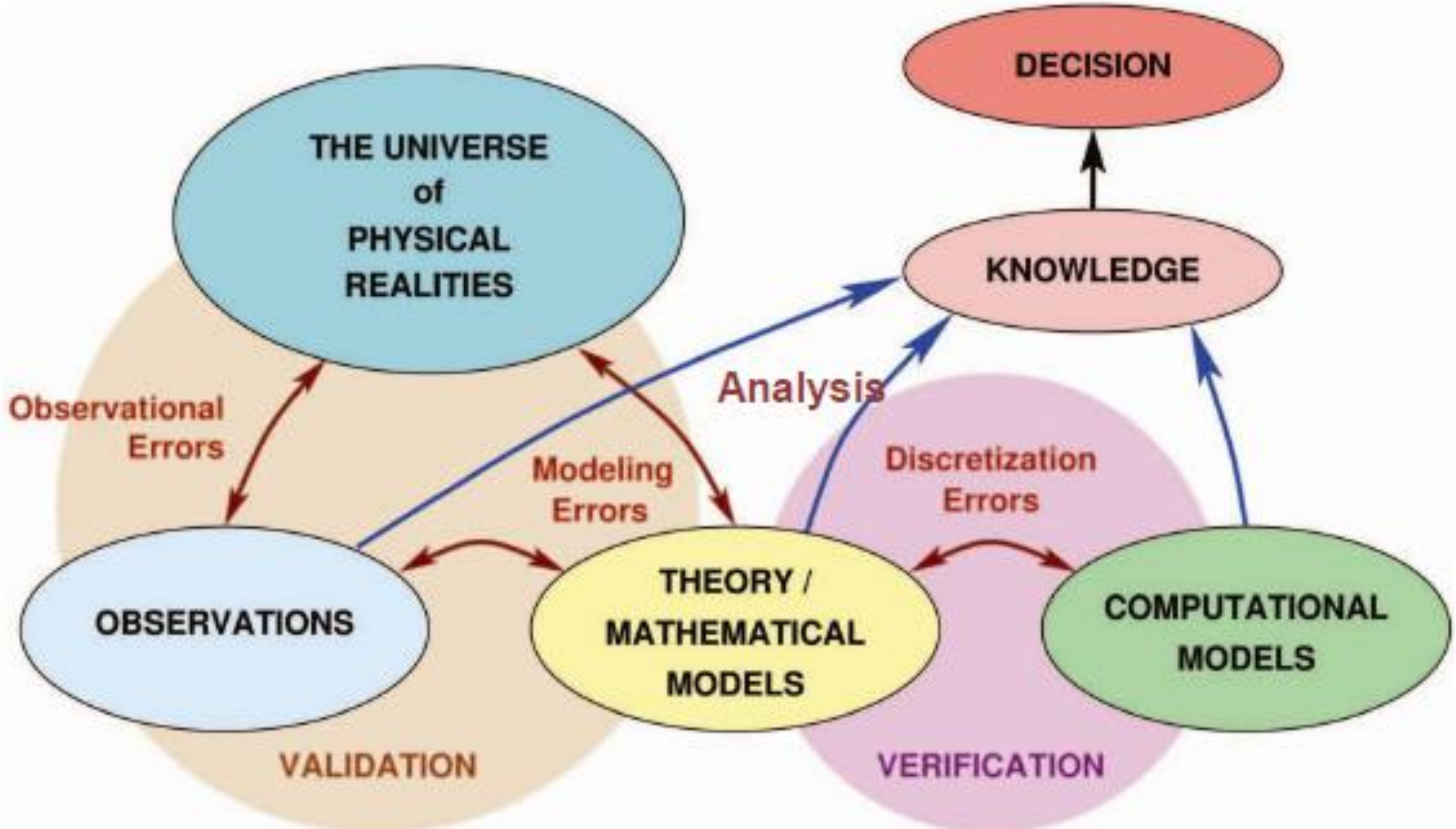
Leads to an increasing focus on VVUQ
Verification **V**alidation and **U**ncertainty **Q**uantification

DOE NNSA has promoted work on this… but

-- "VVUQ turned out to a little bit harder than we thought." PSAAP meeting 2011

Credit: M. Pilch.
Source: Weirs SANDIA

Verification and Validation



We validate mathematical models and verify the software that implements them

Source: Oden et al. SIAM News

DOD in 1994 introduced emphasis on accuracy

Verification Validation and Uncertainty Quantification

Model Validation	Assess physics model against experimental data
Code Verification	Assess algorithms and their implementation vs. exact solutions
Solution Verification	Estimate computational (discretization) error in numerical solution
Sensitivity Analysis/ Uncertainty Quantification	Assess sensitivity or uncertainty of answer to input parameters Aleatory uncertainty – randomness in model or parameters Epistemic uncertainty – due to lack of knowledge.

MSME Collaborative Plans

- Regular meetings

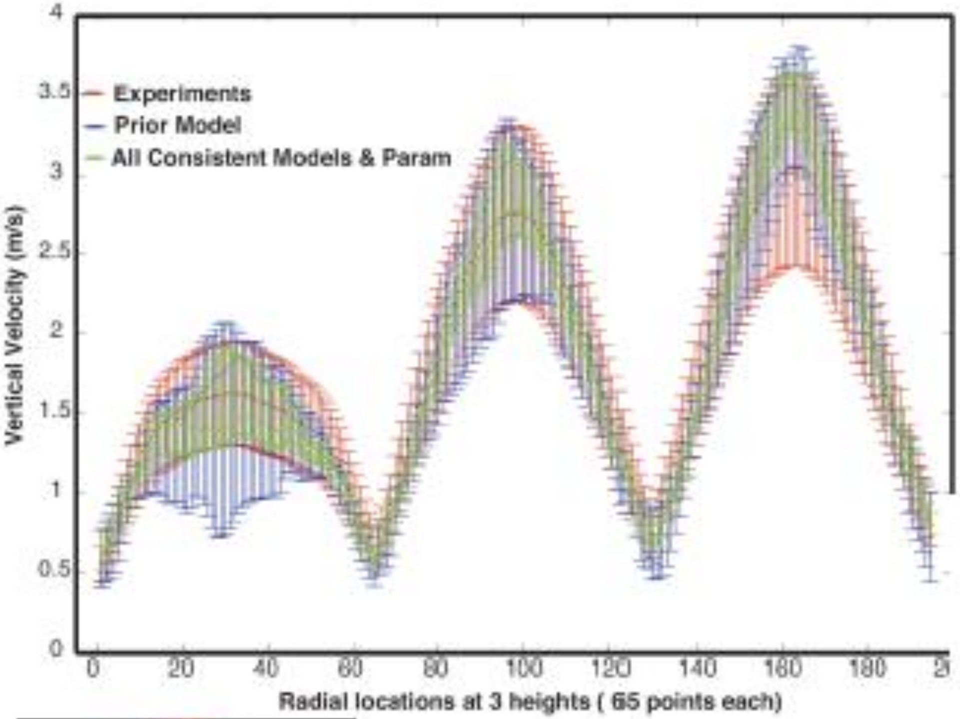
- Regular visits between ARL and Consortium, in both directions
  - Faculty/ARL SME Staff rotations
  - Short term and Long term visits, internships, part-time work at ARL for Phd's, postdocs, students at ARL

- Development of computational infrastructure for sharing data

- Establish collaborative space, both at Consortium and at ARL
- Establish collaboration between MSME, MEDE and ARL Enterprise in cross-cutting areas

- Educational efforts
  - Seminar series (one credit hour each) at BU, UU and RPI
  - Training in computational modeling and parallel computing
    - Boston University Scientific Computing and Visualization group
- MSME Corporate Partnership Program - currently ~50 members

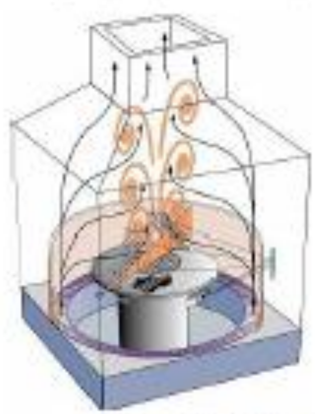
VVUQ State of the Art with Utah Uintah Buoyant Helium Plume Model



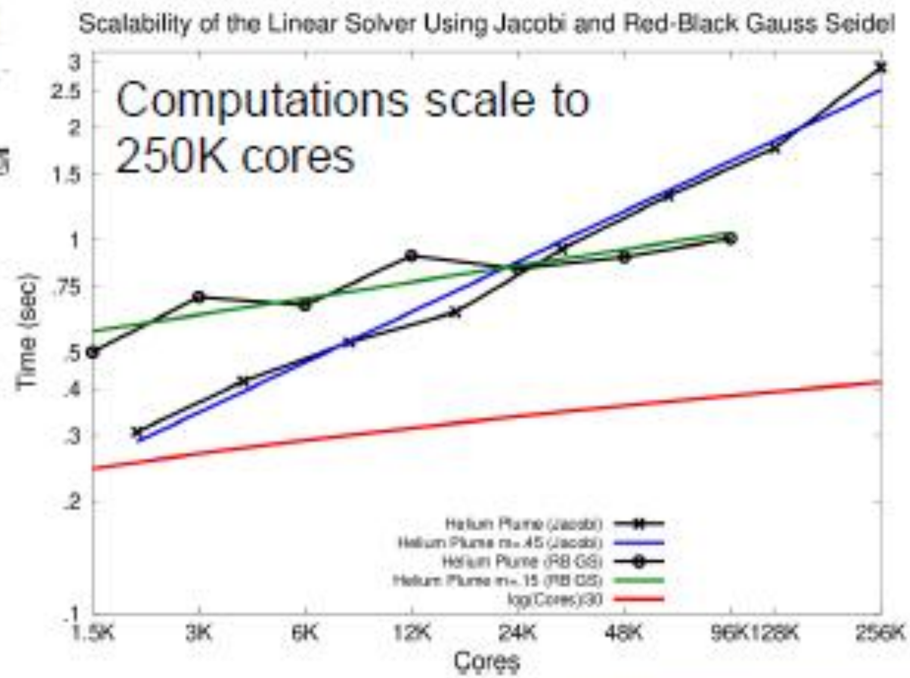
Red is experimental uncertainty

Blue is uncertainty region from simulation

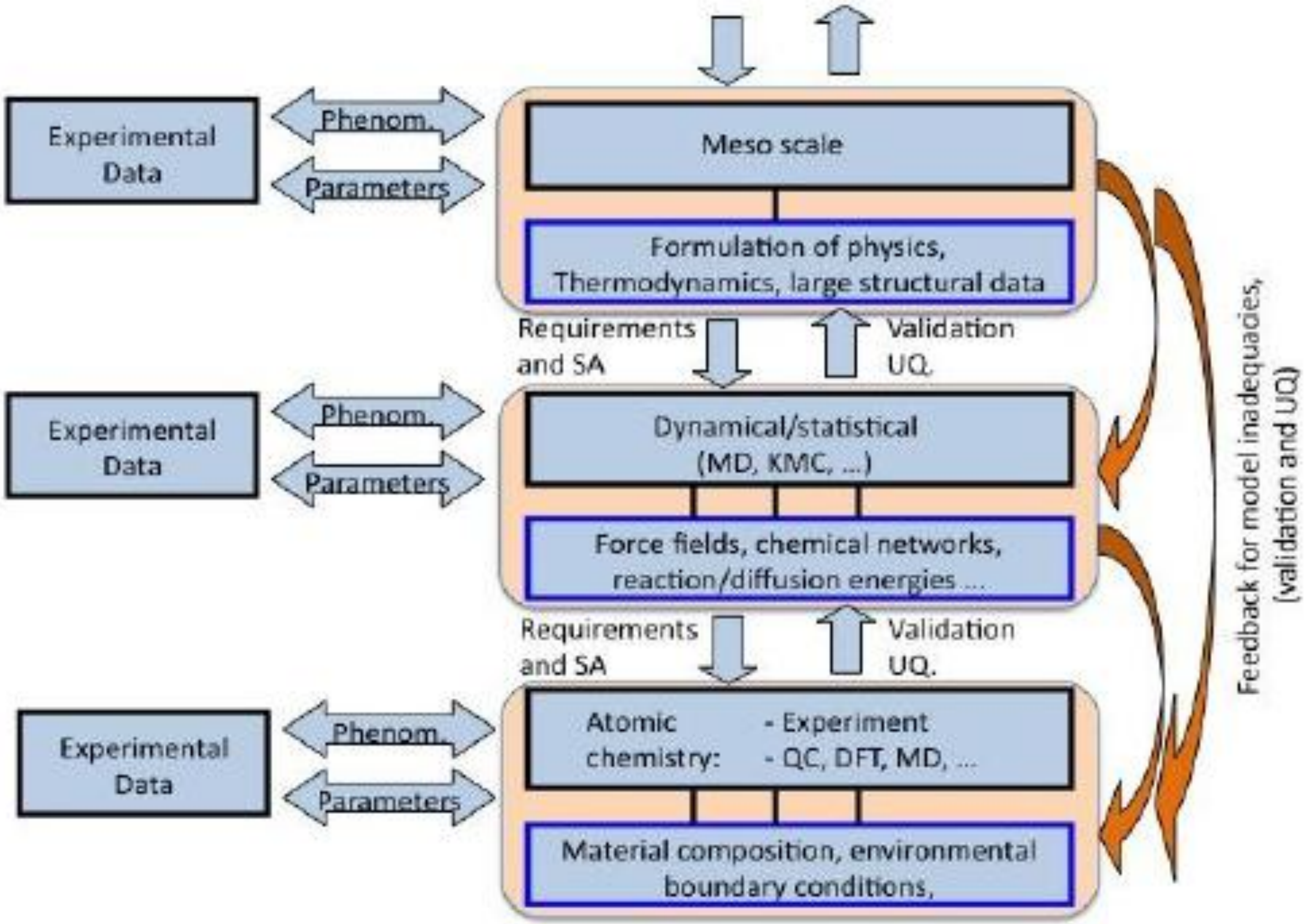
Green is uncertainty in vertical velocity consistent with experimental data and input parameters



Sources: Smith Schmidt



VVUQ in a Multiscale World



We need to understand sensitivity of meso scale simulation to e.g. DFT

Source: P.A. Schultz, SAND2011-9257

Area A: Electrochemical Energy Devices

Projects: **A1 – Lithium Ion Batteries**
A2 – Alkaline Membrane Fuel Cells

Materials Design:

Dmitry Bedrov– molecular and coarse-grained simulations
Adri van Duin – reactive molecular simulations
Tim Kaxiras – multiscale modeling and ab initio methods
Valeria Molinero – molecular and coarse-grained simulations

Crosscutting Efforts:

Martin Berzins – continuum level modeling, computational infrastructure
Mike Kirby – uncertainty quantification and coarse-graining algorithms
George Karniadakis– uncertainty quantification in multiscale modeling
Giulia Galli –ab initio density functional calculations

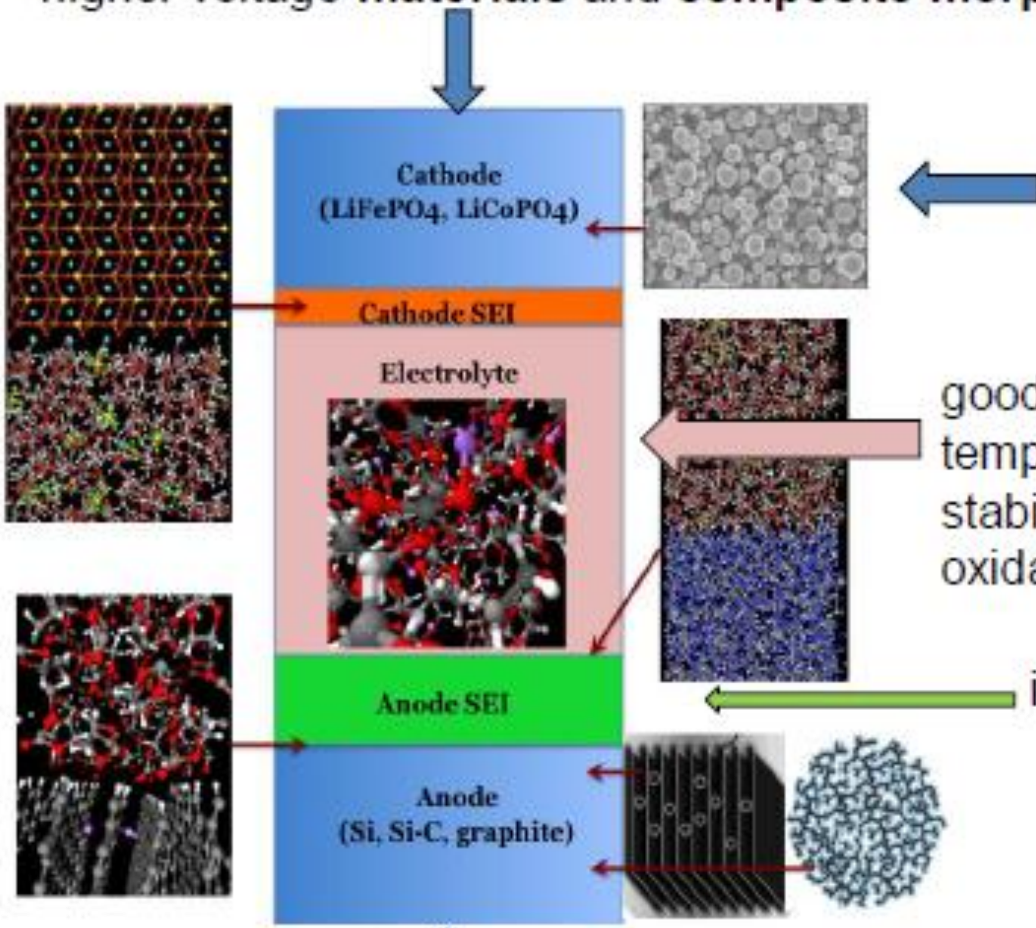
ARL Members:

Oleg Borodin, Richard Jow, Cynthia Lundgren, Kyle Grew, Deryn Chu

Project A1: Lithium Ion Batteries an inherently multiscale problem

Next generation needs:

higher voltage **materials** and **composite morphologies**



a **cathode passivation layer** that allows for high lithium mobility

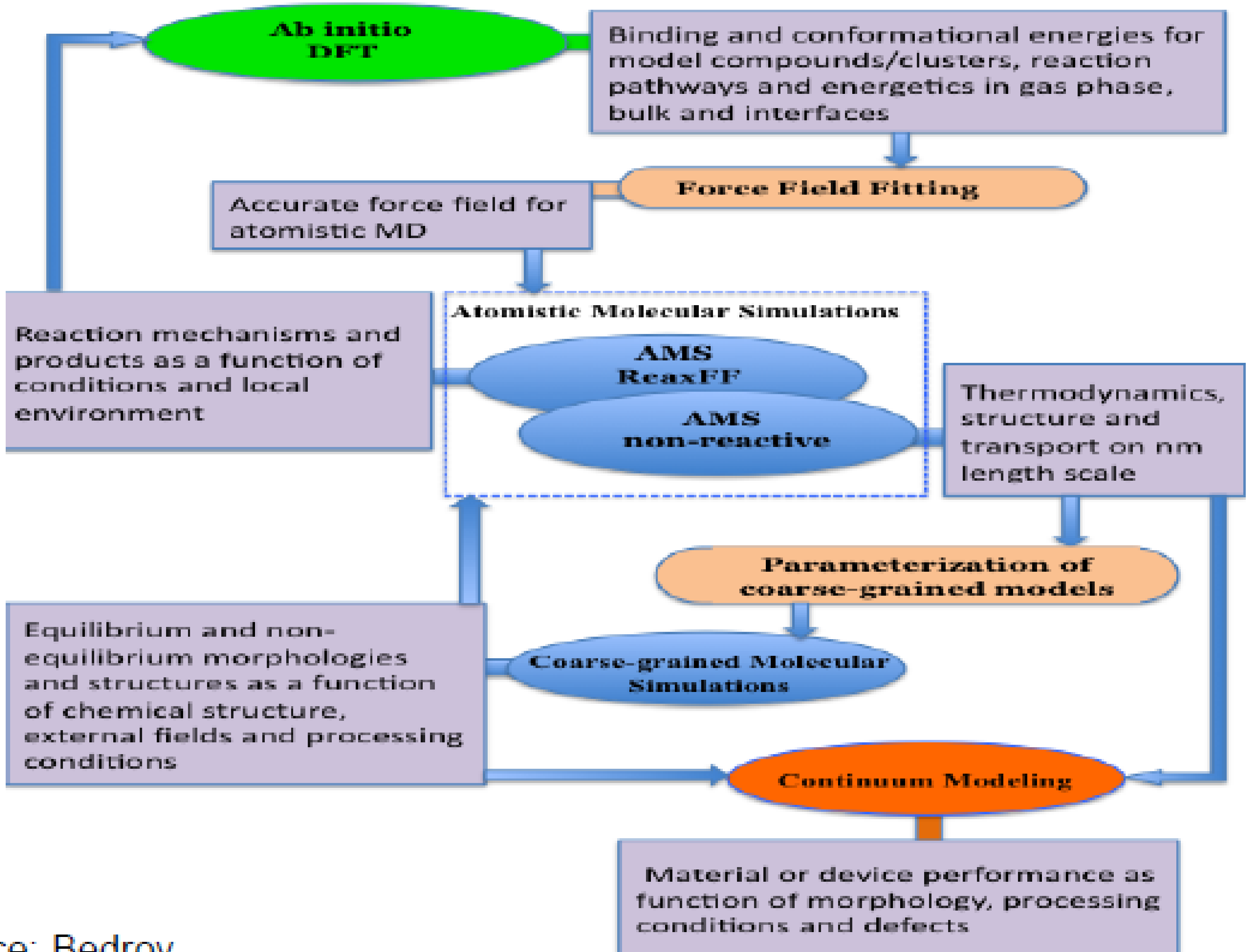
good lithium conduction over a wide temperature range and is stable and/or stabilized by interfacial layers (SEI) from oxidation and reduction

improved conductivity and mechanical integrity;

increased lithium storage capability

Source: Bedrov

Project A1 Multiscale Approach



Source: Bedrov

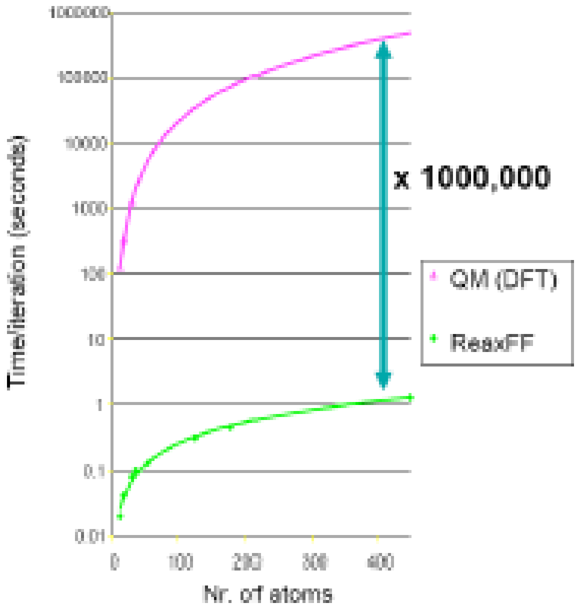
MSME CRA Area Overview

Area A : Two – Year Goals:

- Accurate molecular simulations of electrochemistry (ReaxFF or/and DFT)
- Multiscale modeling of molecular self-assembly (SEI, alkaline membrane)
- UQ-driven methodologies for coarse-graining and scale bridging
- Validation & Verification of selected methods and models.
- Computational framework for multiscale and multiphysics modeling (Uintah)

Five – Year Goals:

- Tools for high through put screening of materials
- Virtual design of advanced novel materials
- Strategy and tools development to address processing and fabrication conditions



Source: Bedrov, van Duin

Area B - Hybrid Photonics Materials

Projects:

- B1 – Material Modeling for Multi-Spectral Detectors
- B2 – Material Modeling for Light Emitters
- B3 – Defects, Interfaces and Dislocation Studies
- B4 – Plasmonics and Metamaterials

Organizational Team Members:

- Enrico Bellotti (Area Lead)
- Luca Dal Negro
- Martin Herbordt
- Michael Shur
- Efthimios Kaxiras
- Francesco Bertazzi
- Giuseppe Vecchi
- Giulia Galli

ARL Team Members:

- Michael Wraback
- Sergey Rudin
- Greg Ruppert
- Ken Jones
- Randy Tompkins
- Meredith Reed

Source: Bellotti

CDE3M THE UNIVERSITY OF UTAH Rensselaer BOSTON UNIVERSITY ARL

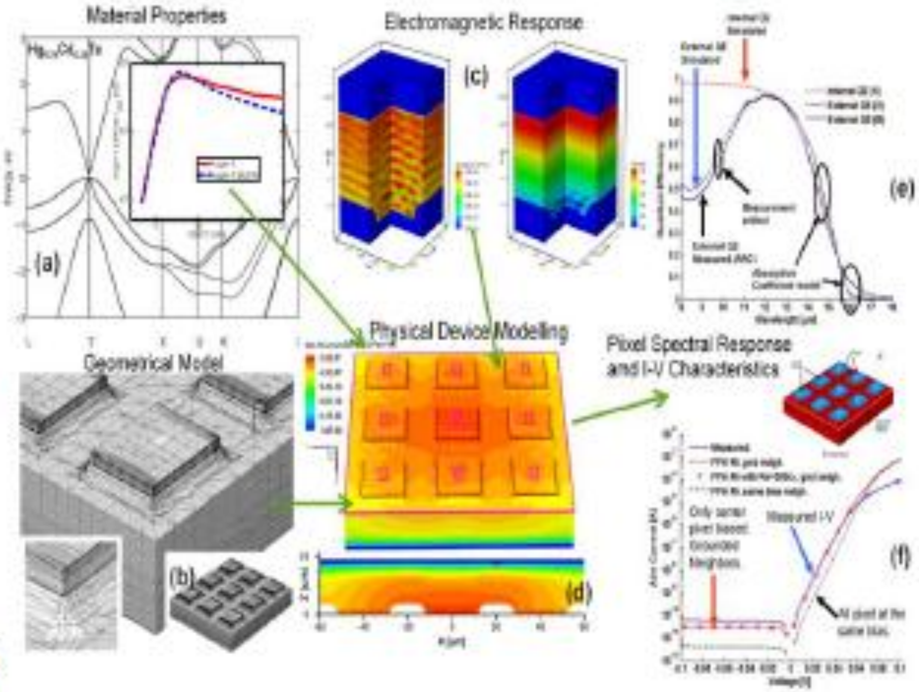
Area B – Hybrid Photonics Materials Summary

State of the art material + simulation methods for:

B1 - Material Modeling for Multi-Spectral Detectors: next generation of materials and device structures for detectors e.g high operating temperature IR for night vision. Year 2 goal :Comprehensive microscopic models of III-Nitrides complex alloys to be used in device simulation.

B2 - Material Modeling for Light Emitters: High efficiency LEDs for lighting applications and UV LEDs for bio-chemical threat detection. Comprehensive microscopic model of the non- radiative and radiative processes in light emitters structures

Multiscale Modeling for IR Materials and Pixel Arrays Models



Source: Bellotti

Area B – Hybrid Photonics Materials - 3 year Goals

B3 - Defects, Interfaces and Dislocation Studies:

Comprehensive **microscopic behavioral models of defects and dislocations in GaN and AlGaN for device simulation – Year** 2 **goal:**
understand /engineer the effects of materials' non-idealities on power electronics and optoelectronics devices.

B4 – Plasmonics and Metematerials:

engineer materials with novel electromagnetic functionalities. E.g for UV radiative rate engineering. enhanced light-matter coupling. **Year 2 goal**:
Design the first UV plasmonic III-nitrides lasers and LEDs structures with controllable radiation rates, far-field profiles and emission time dynamics.

- All projects -– Transfer simulation tools to ARL for evaluation and engage in– V&V procedures
- 5 years goals also defined

Source: Bellotti

Area C: Heterogeneous Metamorphic Electronics

Projects:

- C1 – Graphene Based Electronics
- C2 – Heterogeneous systems for THz Electronics
- C3 – Thermal Transport in Heterogeneous systems

Organizational Team Members:

- Michael Shur (Area Lead)
- V. Meunier
- S. Nayak
- P. Keblinski
- E. Bellotti
- F. Liu,
- Giulia Galli
- T. Reinecke

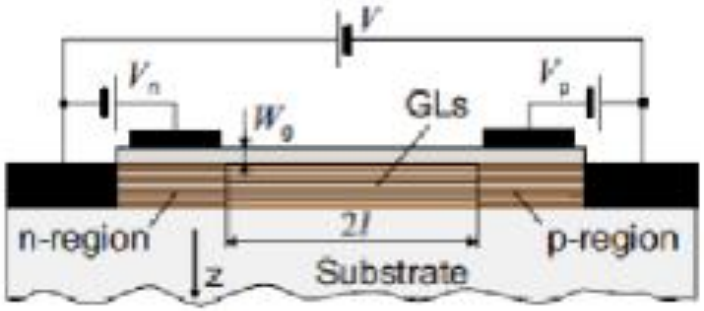
ARL Team Members:

- T. O'Reagan
- S. Rudin
- F. Crowne
- M. Wraback
- M. Dubey

Area C: Heterogeneous Metamorphic Electronics

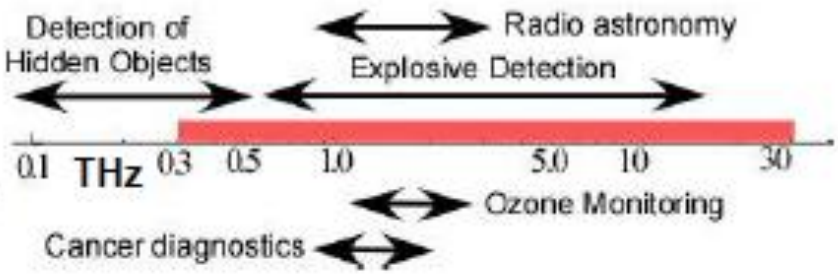
C1. Graphene Based Electronics

2D-crystals have enormous advantage for sensing applications (going beyond CMOS)



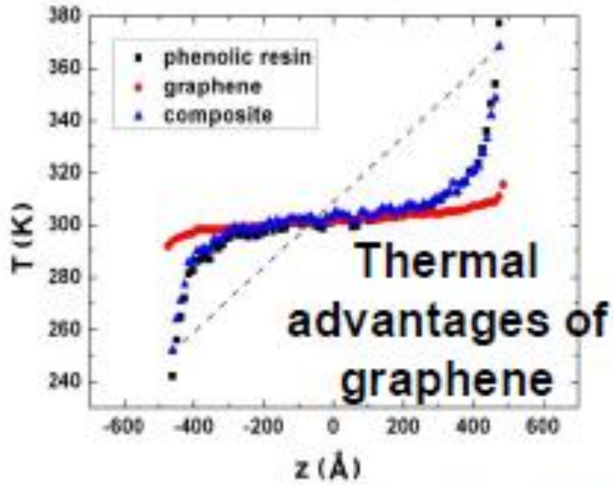
C2. Heterogeneous systems for THz Electronics

Heterogeneous systems may help close famous THz gap opening applications in cancer detection, home land security, etc



C3. Thermal Transport in Heterogeneous systems

Thermal transport determines an ultimate limit for performance of most semiconductor devices and circuits



Area C: Heterogeneous Metamorphic Electronics

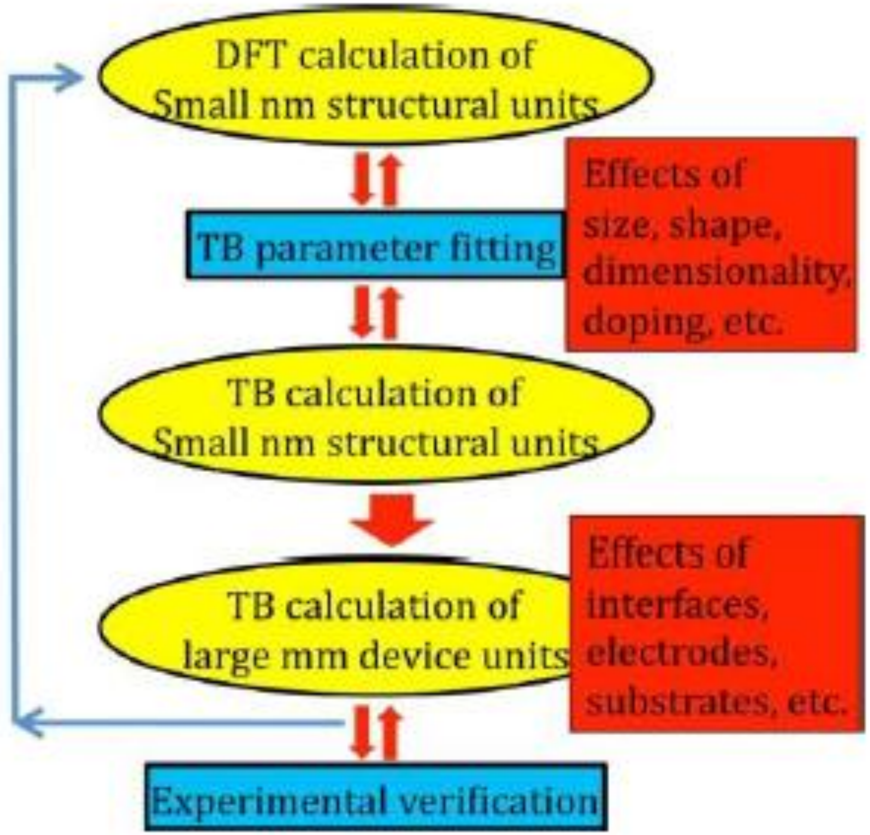
Technical Challenges

Task C1-1: Modeling of graphene transistors (**Shur**) using DFT and Tight Binding methods

Task C1-2: Transport properties of graphitic nanoribbons attached to metallic electrode (Iron). (**Meunier**)

Task C1-3. Role of dielectrics and substrates in graphene electronics (**Nayak**)

Task C1-4. Modeling of graphene hetero-layer junctions and design of flexible keypad (**Liu**)



Multiscale modeling for Graphene-based Electronics

Area C: Heterogeneous Metamorphic Electronics

3-year goals

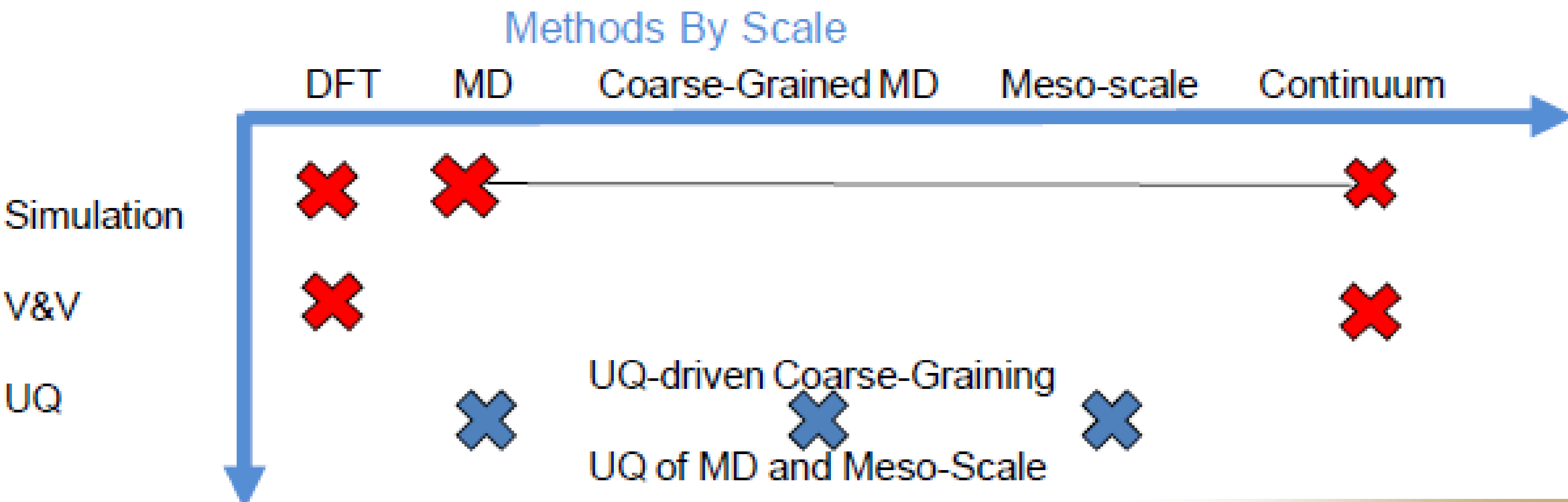
Thrust	Task	Goal
C1. Graphene Based Electronics	C1-1: Modeling of graphene transistors (**Shur**)	Compact graphene transistor model
	C1-2: Transport properties of graphitic nanoribbons (**Meunier**)	First-principles modeling of realistic interface with metallic nanoelectrodes
	C1-3. Role of dielectrics and substrates in graphene (**Nayak**)	Role of dielectrics and substrates on electronic structure of graphene systems
	C1-4. Modeling of graphene hetero-layer junctions (**Liu**)	
C2. Heterogeneous systems for THz Electronics	C2-1: Theory of THz plasmonic graphene laser (**Shur**)	Model of THz plasmonic graphene laser
C3. Thermal Transport in Heterogeneous systems	C3-1: Molecular dynamics simulations of thermal transport (**Keblinski, Galli, Bellotti, Reinecke**)	Predictive models of thermal conduction as a function of defect type, density and interfacial structure and bonding

Area D: Cross-Cutting Themes

Uncertainty Quantification (UQ) / Coarse-Graining
Software Infrastructures: UintahX
Density Functional Theory (DFT)

Team Members:

- Mike Kirby (Area Lead) – **Algorithms VVUQ**
- Martin Berzins – **Adaptive Meshing Petascale and Exascale Computing, Verification and Error estimation**
- Giulia Galli – **DFT Development and simulation**
- George Karniadakis – **gPC UQ Methodology and Multiscale Bridging**



Predictive modeling of multiple properties based on first principles calculations

Classical Molecular Dynamics (MD):

Ground State properties : Structural, dynamical and transport properties

Ab-initio MD using Density Functional Theory (DFT)

Ground State properties : Structural, electronic, some thermodynamic and dynamical properties

Excited State properties
- Many Body Perturbation Theory: Spectra, Correlation energies

Thermodynamic properties
- Effective Hamiltonians for Monte Carlo simulations : Defects in solids and entropy

Vibrational Properties
- DFT-perturbation Theory: IR and Raman Spectra

Transport properties
- Boltzman equation: Heat transport

Excited State properties → Multiscale electromagnetic simulations

DFT Reduces intractable many body problem of interacting electrons to a tractable computational problem of non-interacting electrons moving within an effective potential via Kohn-Shan eqn

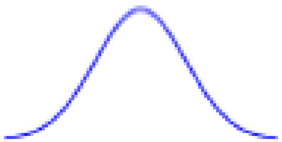
Source: Galli

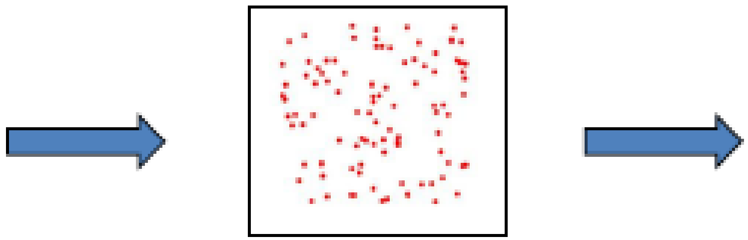
Stochastic Engineering and Uncertainty Quantification

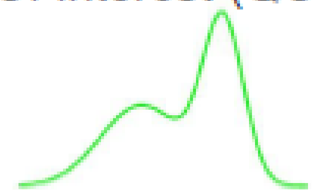
Inputs:
- Initial conditions
- Boundary conditions
- Model parameters

Monte Carlo
Sampling of Solver

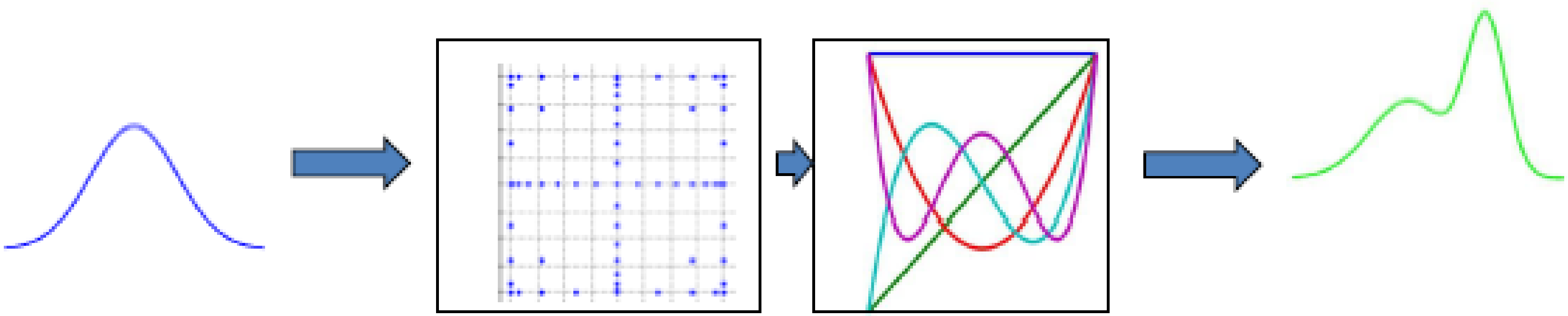
Distribution of
output quantity
Of interest (QOI)







Input probability distribution
for parameters



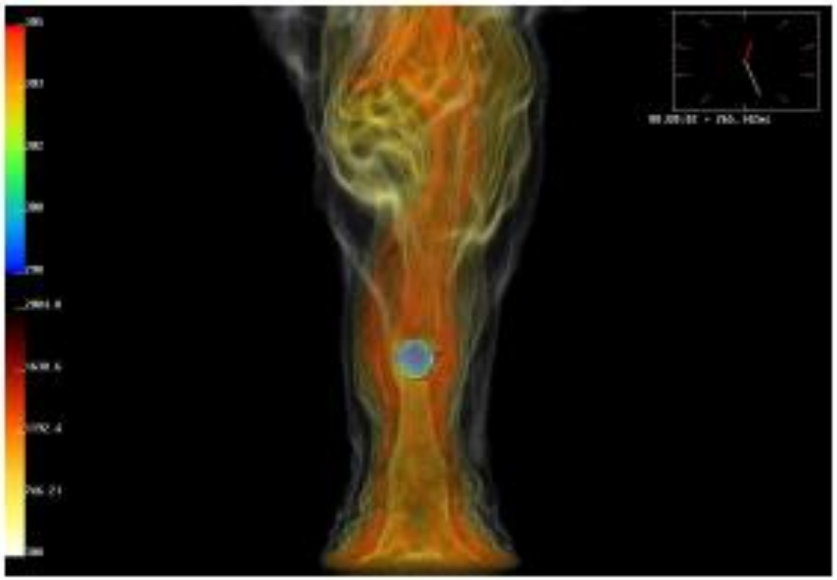
Judicious sampling
of solver solution
at quadrature points

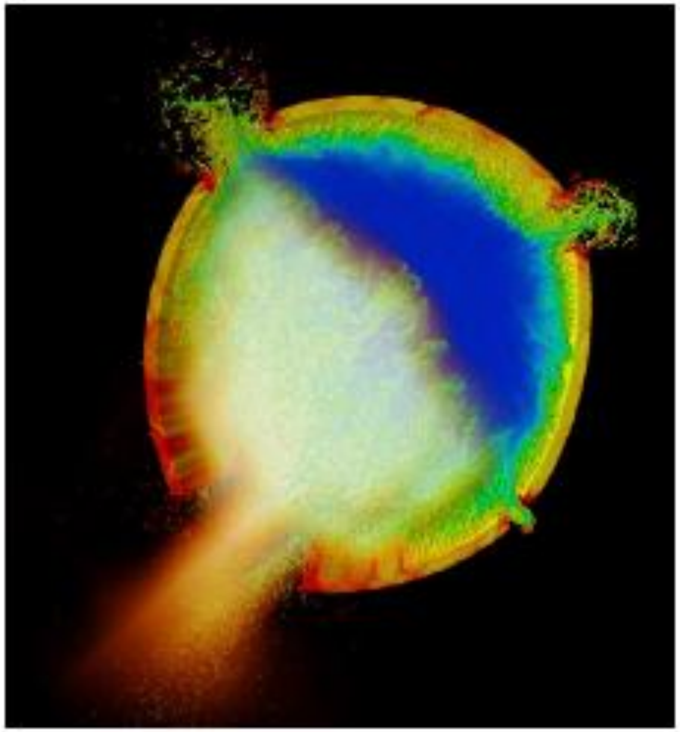
Use polynomial chaos
representation of uncertainty
Generalized Polynomial Chaos

Source: Witteween

UintahX Software and Adaptive Mesh Refinement

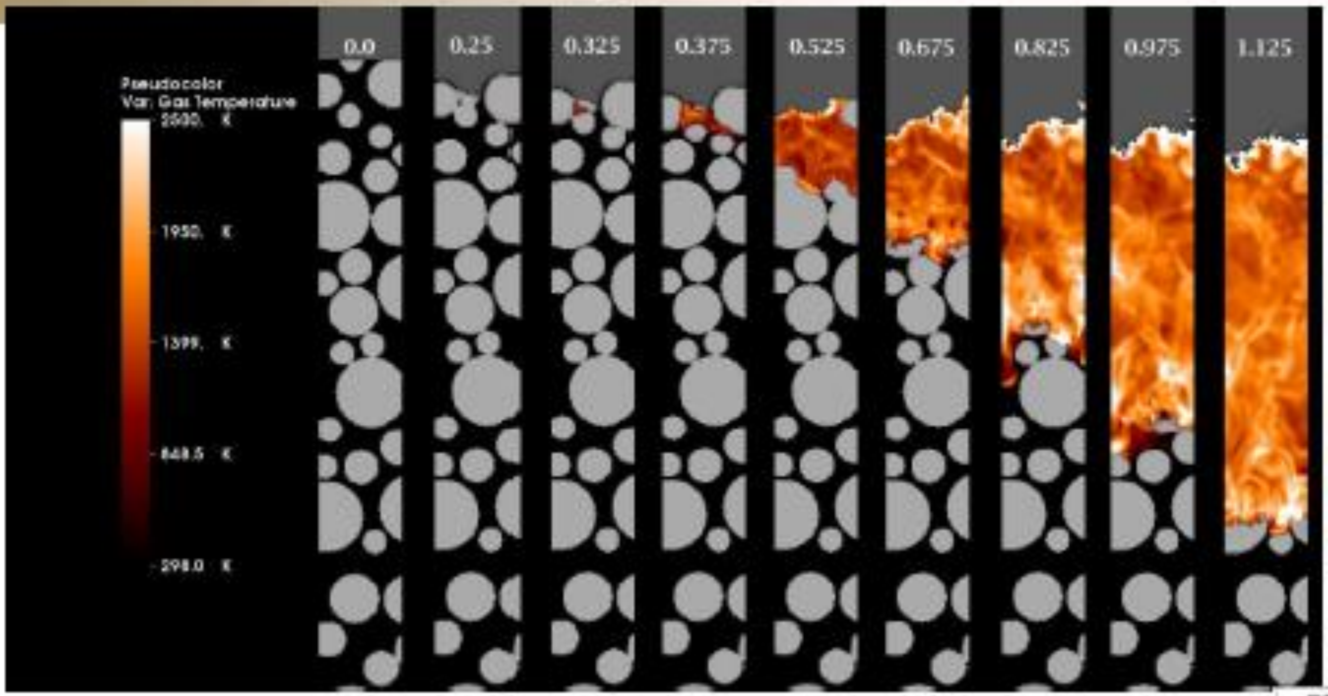
Steel container containing PBX 9502 in A pool fire



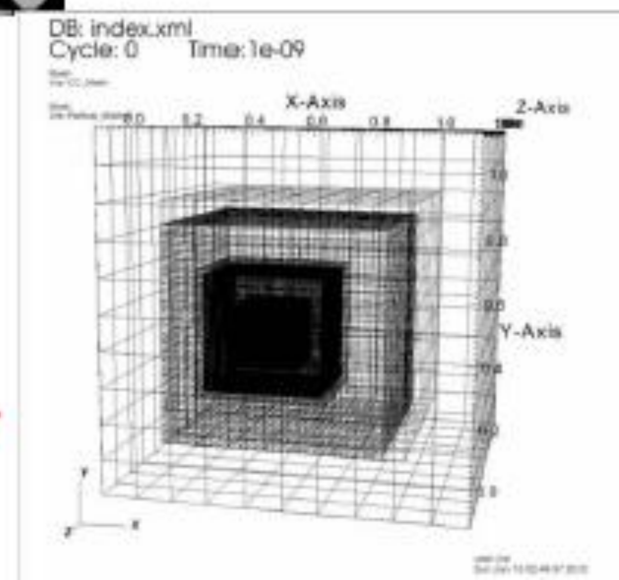


Runs on CPUs GPUs Adaptive Meshing Different Physics on different meshes

UintahX Software on Deflagration Problem



Fluid-structure interaction and AMR Scalable to 256K cores



Different physics on finest mesh – model for MD continuum coupling.

Extend Uintah to include MD on finest meshes

We need to design algorithms and solvers for at least the next decade With 1000x increase in compute power

Source: Peterson

Area D: Cross-Cutting Themes

Technical Challenges:

- **Galli:** Application and development (inc. V&V) of DFT for electrochemical materials of interest to ARL.
- **Kirby**: Exploiting computational savings and accuracy enhancement available through the gPC framework for accomplishing UQ-driven force matching in coarse-graining.
- **Karniadakis**: Accomplishing the first ever attempt at UQ of MD and Mesoscale Modeling.
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- **Berzins:** Incorporation of particle-to-particle (direct) interactions into the Uintah Framework for accomplishing MD + Continuum Modeling. Verification of MPM and MD codes in coupled mode.

Project A1: Lithium Ion Batteries

Design of new batteries has to bridge molecular level understanding (Li^+ transport, electrochemistry at interfaces, etc.) and the underlying macroscopic structure of composite electrodes and requires:

(i) Implementation and validation of hierarchical multiscale modeling approaches with bidirectional bridging.

(ii) Enhancement of models and methods to accurately capture all key electrochemical and thermophysical processes.

(iii) Implementation of UQ-driven coarse-graining and scale bridging methodologies.

Will build on existing multiscale modeling of electrode materials

Source: Bedrov

Infrastructure & Capabilities

Electro Optics & Photonics

- Time-Resolved Infrared Spectroscopy Facility
- MOCVD, MBE semiconductor growth
  - Indium Phosphide
  - Gallium Nitride
  - Gallium Antimonide
  - Lead Tin Telluride
  - Mercury Cadmium Telluride
  - Gallium Arsenide

Microanalysis

- SEM/EDXS
- SIMS
- HR TEM
- XRD
- Auger/XPS
- AFM
- FIB
- Micro Raman

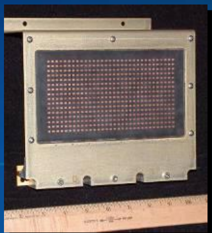
Specialty Electronic Materials and Sensors Cleanroom

- E-Beam Lithography System
- i-line Lithography
- Lithography Stepper (optical)
- In-Process Material and Device Characterization
- Piece Part to 6" Wafer Capable
- RF Range Facility
- E/B – Field Sensor Suite
- Metal & Dielectric Deposition
- LPCVD High Temperature Processing and Wafer Bonding
- RIE/ICP

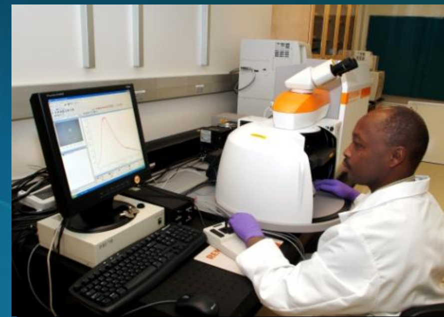
Power & Energy

- Reformer Lab
- Power Conditioning Lab
- Energy Storage Labs
- Micro Power Lab
- Power MEMS

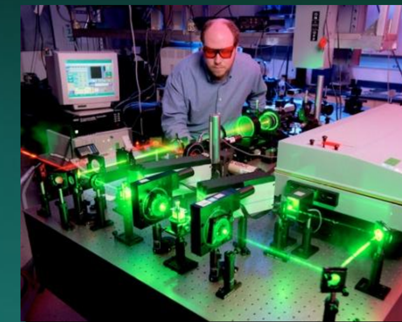
Sensors: Infrastructure & Capabilities



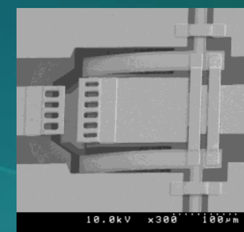
Radar, Antenna & MFRF



Spectral dissection of bacteria and thin-films



Non-linear Optics



NEMS & MEMS PZT

RF Material & Devices

Electric Field Cage for sensor evaluation

Device Fabrication Advanced RF Technology

DC-40GHz environmental cryogenic I/V probe station

Piezoelectric Sputtering for MEMS and communication devices

Electronic transport characterization in nano-scale structures

III-V Etching for optical device fabrication

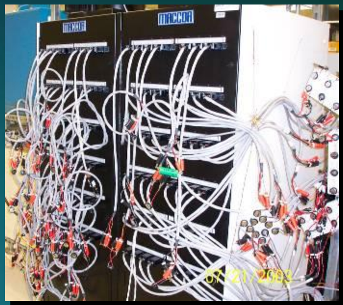
Device Fabrication Electro-Optics

Power & Energy: Infrastructure & Capabilities

Jet Vapor Deposition

Dry Room for electrochemical cell preparation

Single and multiple battery cell evaluation laboratories

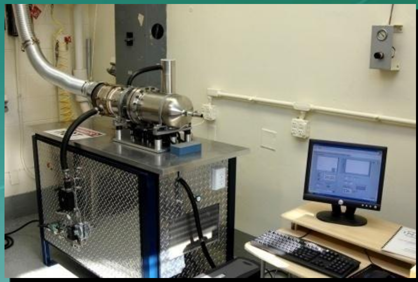


Electric Drive

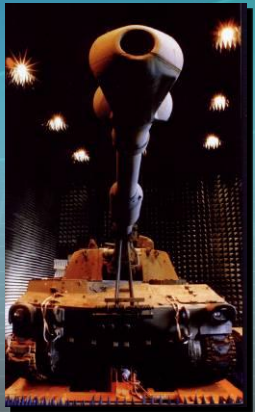
Isomer Battery Laboratory

Power Conditioning Lab

Fuel Cell evaluations

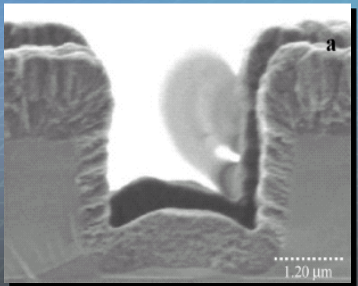


Small Engine Evaluation



High Power RF Anechoic Chamber

Air Gun for high-G evaluation



SiC device stress analysis evaluations

Fuel Cell Powered Robotic Vehicle

Backup